The Structural Chemistry of Energetic Compounds

ONR Annual Report

Oct 1 1983 to Oct 1 1984

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Structural characterization of 12 energetic materials and precursors by x-ray diffraction was performed. The materials examined include: 6,6,10,10-tetranitropentacyclo[5.3.0.$0^{2,5}$.$0^{3,9}$.$0^{4,8}$]decane; 2,6-Diamono-3,5-dinitro-1,4-pyrazine; 4,4,8,8-tetranitro-bicyclooctane; 2,3,4-Trinitropyrrole; 1,3,5-Trinitroso-1,3,5-triazacyclohexane; 3,3-Bis(methyl-nitroaminomethyl)oxetane; 3,3-Bis(nitratomethyl)-oxetane; 3-Methoxy-2,4-dinitro-2,4-diazapentane; Tribenzyltriazawurtzitane; 3-Cyano-4,4,5,5-tetramethylisoxazoline-n-oxide; (OVER)

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5-Aza-6-methoxyiracil; and N-(4-amino-1,2,5-triazolo)-N'-methoxy-trichloroacetamidine. The compounds studied range in density from 1.175 mg/mm^3 (tribenzyl-triazawurtzitane) to 1.856 mg/mm^3 (trinitropyrrole) and four have crystal densities in the range 1.717 to 1.856 mg/mm^3. Originator Supplied Keywords include:

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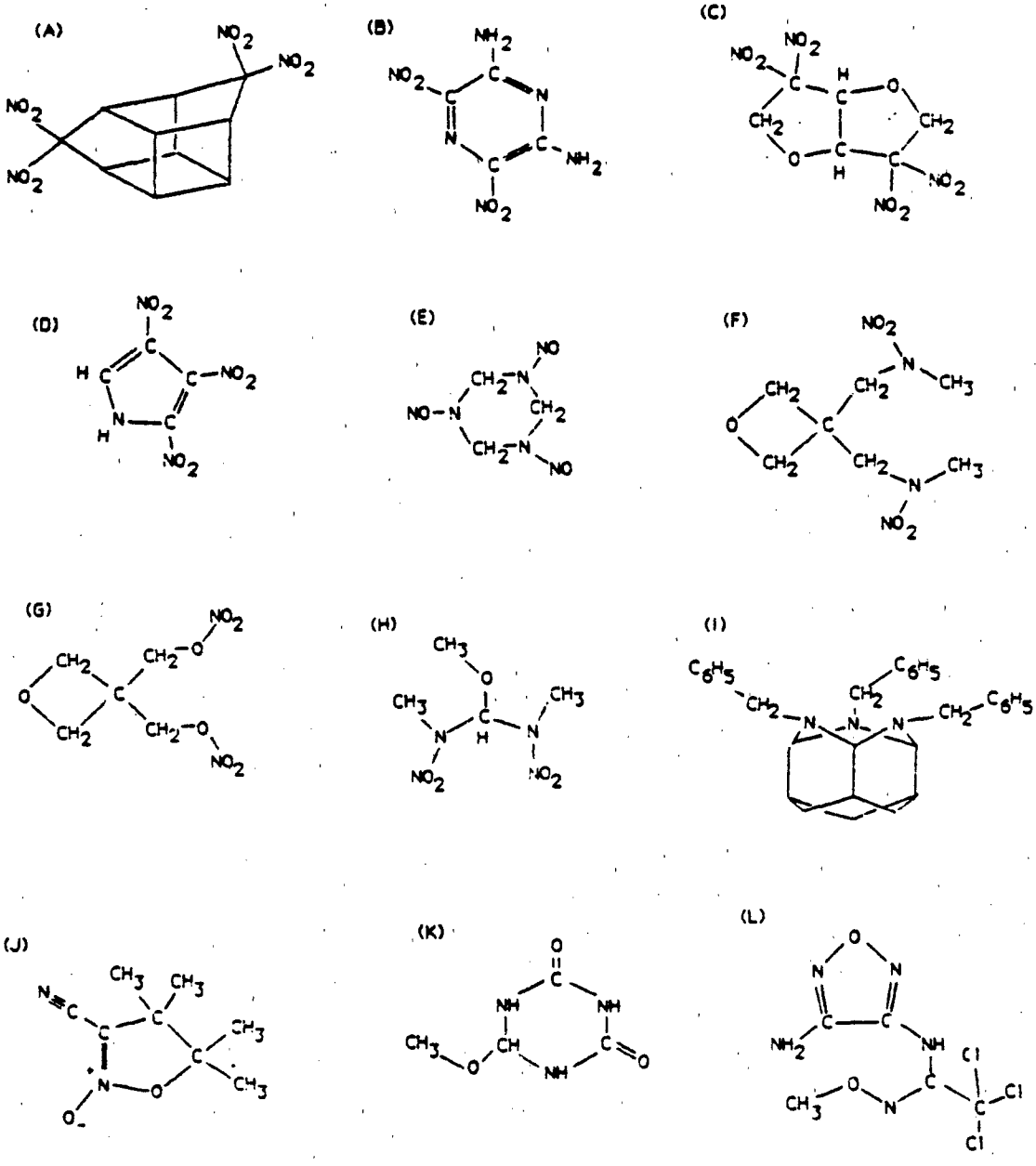


Structural diagrams of molecules included.

Introduction

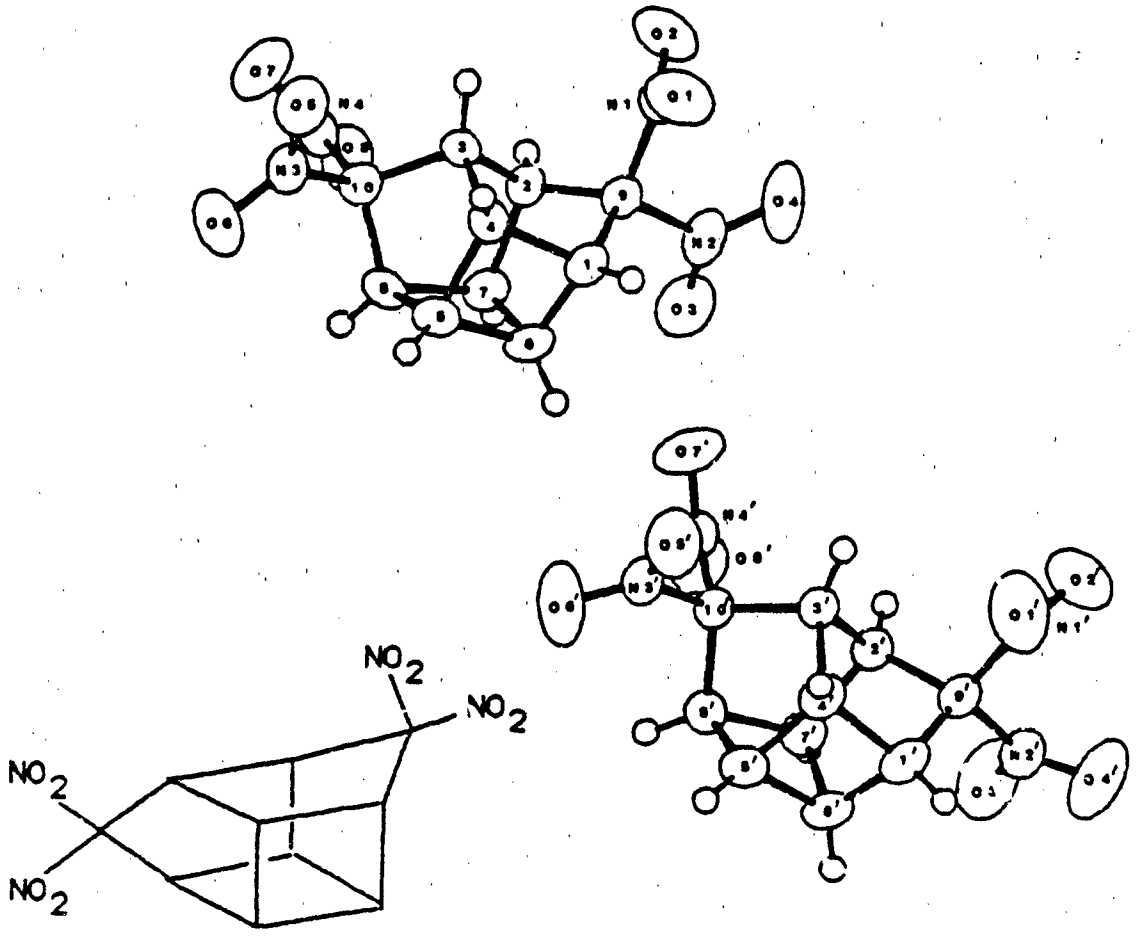
This report summarizes the work conducted under contract No. N0001484-WR24060 for the period Oct. 1 ,1983 to Oct. 1, 1984 under the sponsership of the Office of Naval Research, Code 432P (Dr. R. S. Miller). The task is to provide prompt structural characterization of new energetic compounds, or their synthetic precursors, developed in the ONR energetics materials synthesis program. The results of the investigations also provide structural parameters for energetic groups used to model hypothetical target compounds by methods of conformational energy analysis and quantum chemistry. This work is a continuation of previous work. Results of the examination of twelve energetic materials and precursors are included.

a) Tetranitrobishomocubane

This polynitro cage compound was provided by A. P. Marchand and D. S. Reddy of North Texas State University. The material crystallized in the monoclinic space group Pc, a = 7.751(1)Å, b = 11.500(2) , c = 14.277(2)Å, and β = 108.63(3)°. The calculated density is 1.717 Mg mm^{-3}. In Fig. (1) the two molecules in the asymmetric unit are shown. The primary difference between the two molecules is the orientation of NO_2 groups; corresponding C-C-N-O and O-N-C-N torsion angles have values that differ from one molecule to the other by amounts ranging from 8 to 30°. Bond distances and angles are given in Table (1). The primed molecule in Fig. (1) corresponds to Molecule 2 in Table (1).

There are no unusual intermolecular contacts and no hydrogen bonds, nearest conacts are O(2)'--H(3) = 2.488(33)Å and O(6)--H(3)' = 2.673(31)Å. The molecules pack with the oxygens of Molecule 1 opposing those of Molecule 2. Nearest O--O approaches are in the range of 2.84 to 3.26Å for each of the oxygen atoms in the asymmetric unit.

Fig. (1)



Tetranitrobishomocubane

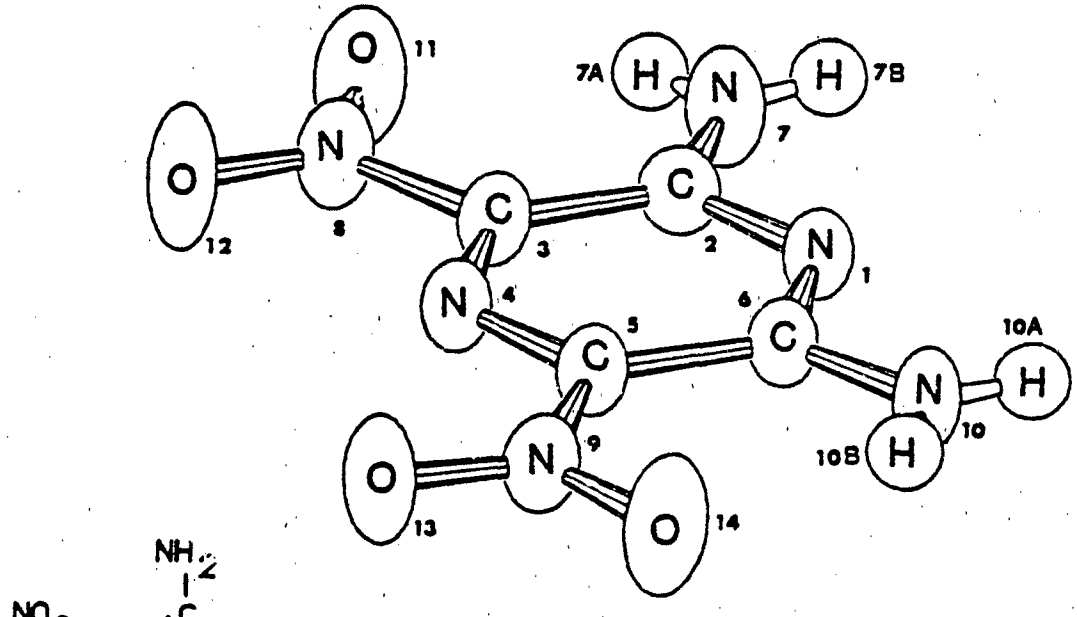
d = 1.717

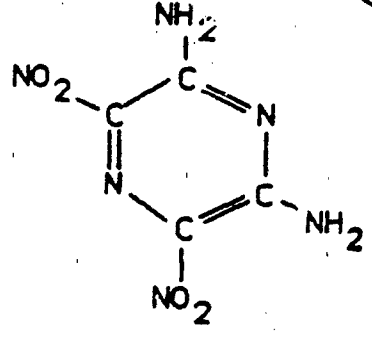
b) 2,6-Diamiro-3,5-dinitro-1,4-pyrazine (ANPZ)

This compound is a very stable di-aza analog of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) and was provided by C. L. Coon of Lawrence Livermore Laboratories. The material crystallized in the monoclinic space group $P2_1/c$, a = 9.030(1)Å, b = 12.977(1)Å, c = 6.405(1)Å, β = 100.76(1)°. The calculated density is 1.803 Mg mm^{-3}. The molecule is shown in Fig. (2) and bond distances, bond angles, and selected torsion angles are given in Table (2) and (3). The molecules of ANPZ are essentially planar with a maximum deviation from a least squares plane through all atoms of 0.07(1)Å. The atom planes are coincident with the crystallographic Z = 1/4 and 3/4 planes with an unusually close interplanar spacing of 3.146Å.

The graphite-like layers which have been observed in the crystal structures of both ANPZ & TATB are held together within each layer by intermolecular hydrogen bonds, and ANPZ, like TATB, decomposes before melting at temperatures greater than 300°C. It is also insoluble in most common solvents. In Fig. (3), which illustrates the hydrogen bonding, two of the hydrogen bonds are bifurcated; i.e., these two hydrogen atoms each participate in one intra- and one intermolecular H-bond. The other two hydrogen bonds are intermolecular with one being long (O--H = 2.49Å). While ANPZ has 2 fewer intermolecular H-bonds and a lower density than TATB, its similar thermal and solubility properties suggest that dipole/dipole and dipole/induced dipole interactions between layers may be important in explaining the extreme stability of this class of materials.

Fig. (2)

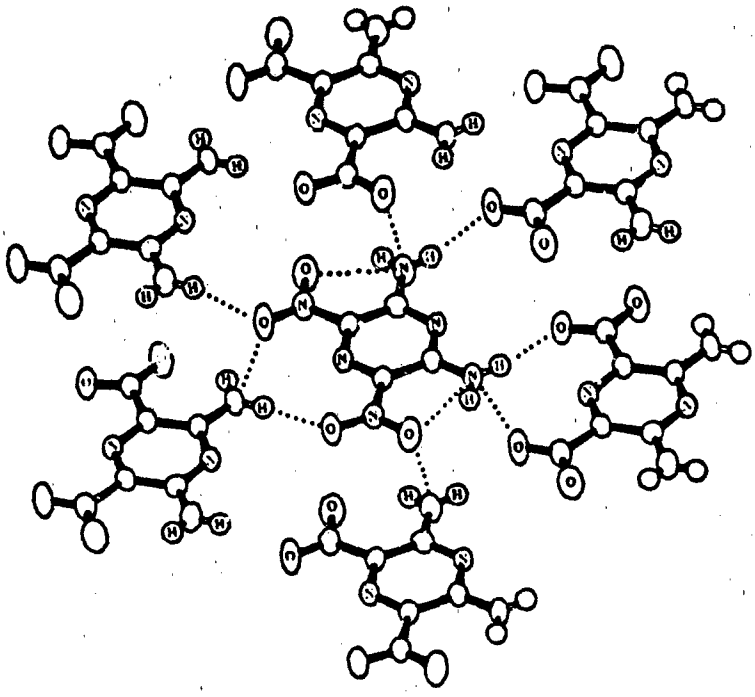




2,6-Diamino-3,5-dinitro-1,4-pyrazine

d = 1.803

Fig. (3)



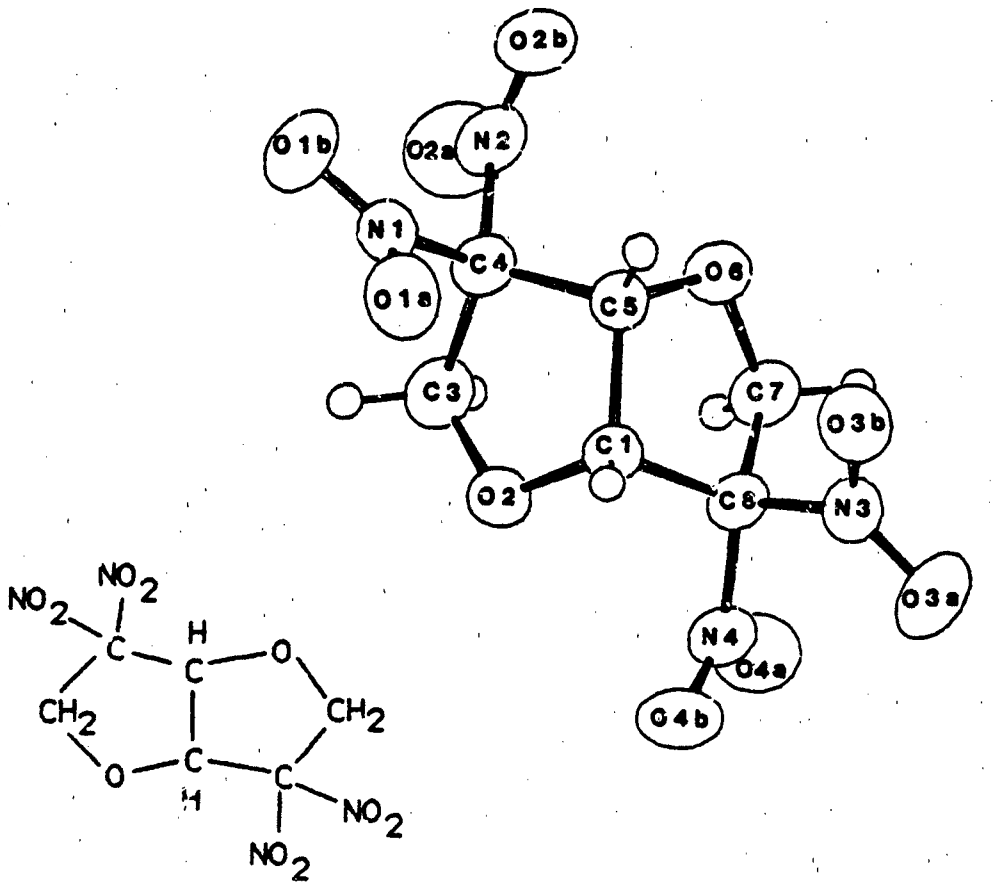
Crystal packing for ANPZ illustrating intermolecular hydrogen bonding

c) 4,4,8,8-Tetranitrobicyclooctane.

This polynitroaliphatic compound was synthesized by K. Baum of Fluorochem, Inc., Azusa, California. The compound crystallized in the monoclinic space group $P2_1$ with a = 9.631(1)Å, b = 11.539(2)Å, c = 10.205(1)Å, and β = 105.31(1)°. The calculated density is 1.786 $M_g\ mm^{-3}$. There are two chemically identical but crystallographically distinct molecules in the asymmetric unit; bond distances and angles for both are given in Table (4). Molecule 1 is shown in Fig. (4). Molecule 2 is similar in conformation, but exhibits a ring-pucker disorder. In approx. 30% of the unit cells, ring atom C(3)' takes an alternate position, C(3)". The dihedral angle between the O(2)'-C(3)'-O(4)' and the O(2)'-C(3)"-O(4)' planes is 68°. The nitro groups bonded to C(4)' also occupy alternate positions. Torsion angle O(1a)'-N(1)'-C(4)'-C(5)' = 23°, while O(1a)"-N(1)"-C(4)'-C(5)' = 35° for the lower occupancy position. The relative orientation of the disordered nitro groups also changes, with the torsion angles O(1a)'-N(1)'-C(4)'-N(2)' = 144.1 and O(1a)"-N(1)"-C(4)'-N(2)" = 92.1°.

There are no unusual intermolecular contacts; nearest contacts are O(1b)'--H(7b) = 2.50Å , O(2b)--H(3a)' = 2.56Å, and O(2b)"--H(5)' = 2.64Å. The nearest nonhydrogen contact is O(2b)'--O(1a)' = 2.73Å.

Fig. (4)



4,4,8,8-Tetranitrobicyclooctane

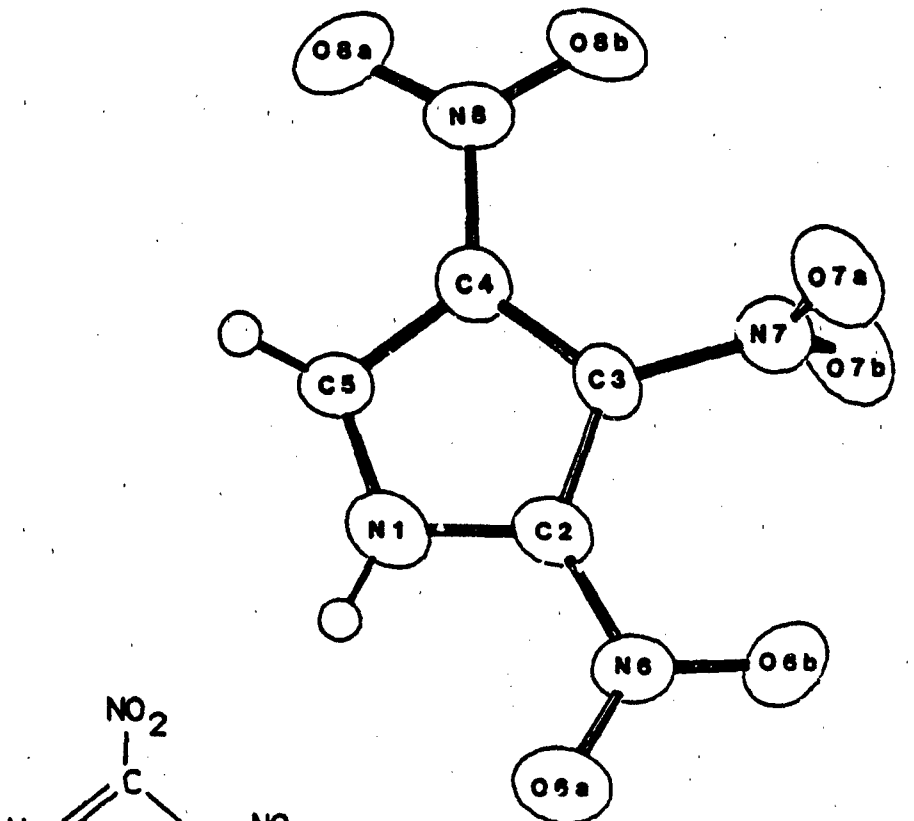
d = 1.786

d) 2,3,4-Trinitropyrrole

This polynitroheterocyclic compound was provided by J. C. Hinshaw of Morton Thiokol. This compound crystallized in the orthorhombic space group $Pca2_1$ with a = 10.113(3)Å, b = 9.686(2)Å, and c = 14.767(3)Å. The calculated density is 1.856 Mg mm^{-3}. One of the two molecules in the asymmetric unit is shown in Fig. (5), and bond distances and angles are given in Table (5). In the crystal the ring nitrogen is in position 1 in both molecules of the asymmetric unit. Interchange of the C and N atoms between the chemically equivalent ring positions 1 and 5, however, affects the residual only modestly. Table (5) gives the bond distances and angles of each of the two molecules in the asymmetric unit as well as the average. The two molecules are observed to have a range of values for the individual bond distances and angles and large standard deviations while the average of the two is closer to the distances and angles normally expected, indicating a disorder with respect to the ring nitrogen site. The pyrrole ring is planar and the 2 and 4 nitro groups are very nearly coplanar with the ring while the plane of the 3-nitro group is perpendicular to the ring.

There are no unusual intermolecular contacts, nearest contacts are H(1)--O(8B)' = 2.34Å and H(1)--O(7B)' = 2.42Å.

Fig. (5)



2,3,4-Trinitropyrrole

d = 1.856

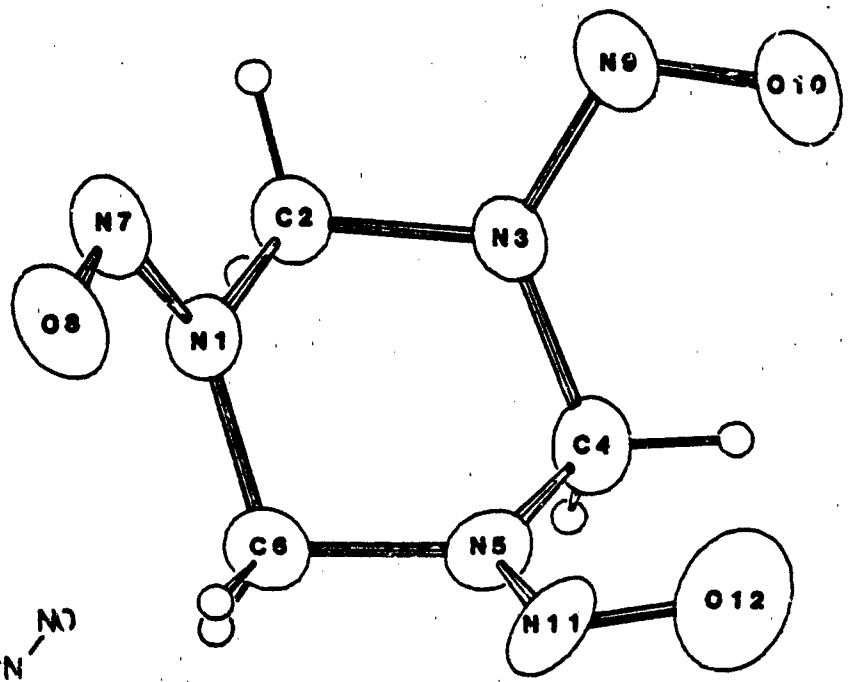
e) 1,3,5-Trinitroso-1,3,5-triazacyclohexane

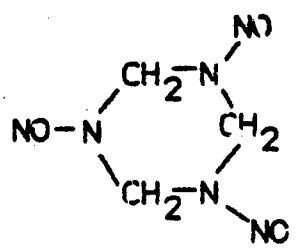
Crystals of this material, commonly known as R-salt, were supplied by J. Boyer of the University of Illincis at Chicago. The observed space group is $P2_1/c$, with a = 9.060(1)Å, b = 6.236(1)Å, c = 12.874(2)Å, and β = 92.47(1)°. The calculated density is 1.573 Mg mm^{-3}. Bond distances and angles are given in Table (6) with the molecular geometry shown in Fig. (6). Not shown in the figure are the disordered atoms. There is a multiple disorder of the nitroso group at N(5) and indications of a disorder of the nitroso group at N(1). The occupation percentages of the nitroso group at N(5) and its two disordered positions, N(11)-O(11), N(11A)-O(11A), and N(11B)-O(11B), are 47%, 28% and 24%, respectively. In both major and minor forms of R-salt, the nitroso groups are all on one side of the chair shaped hexane ring. Aza nitrogens within the ring are pyramidal with the N-N vector making an angle in the range of 8.5 to 13.5° with the plane through the aza nitrogen and its two neighboring ring carbons except for the N(11A)-N(5) vector which is calculated at -2° with respect to the C(6)-N(5)-C(4) plane.

There are no intermolecular contacts, nearest contacts are O(12B)---H(4A, O(12)---H(4A)' = 2.55Å, and O(10)---H(6A) = 2.56Å.

This material was also observed to crystallize in the trigonal space group $R\bar{3}$ when grown from CCl_4 or $CHCl_3$, a = c = 36.340Å, c = 6.089Å, γ = 120°. The solvent which is disordered occupies a channel along the $\bar{3}$ axis.

Fig. (6)





1,3,5-Trinitroso-1,3,5-triazacyclohexane

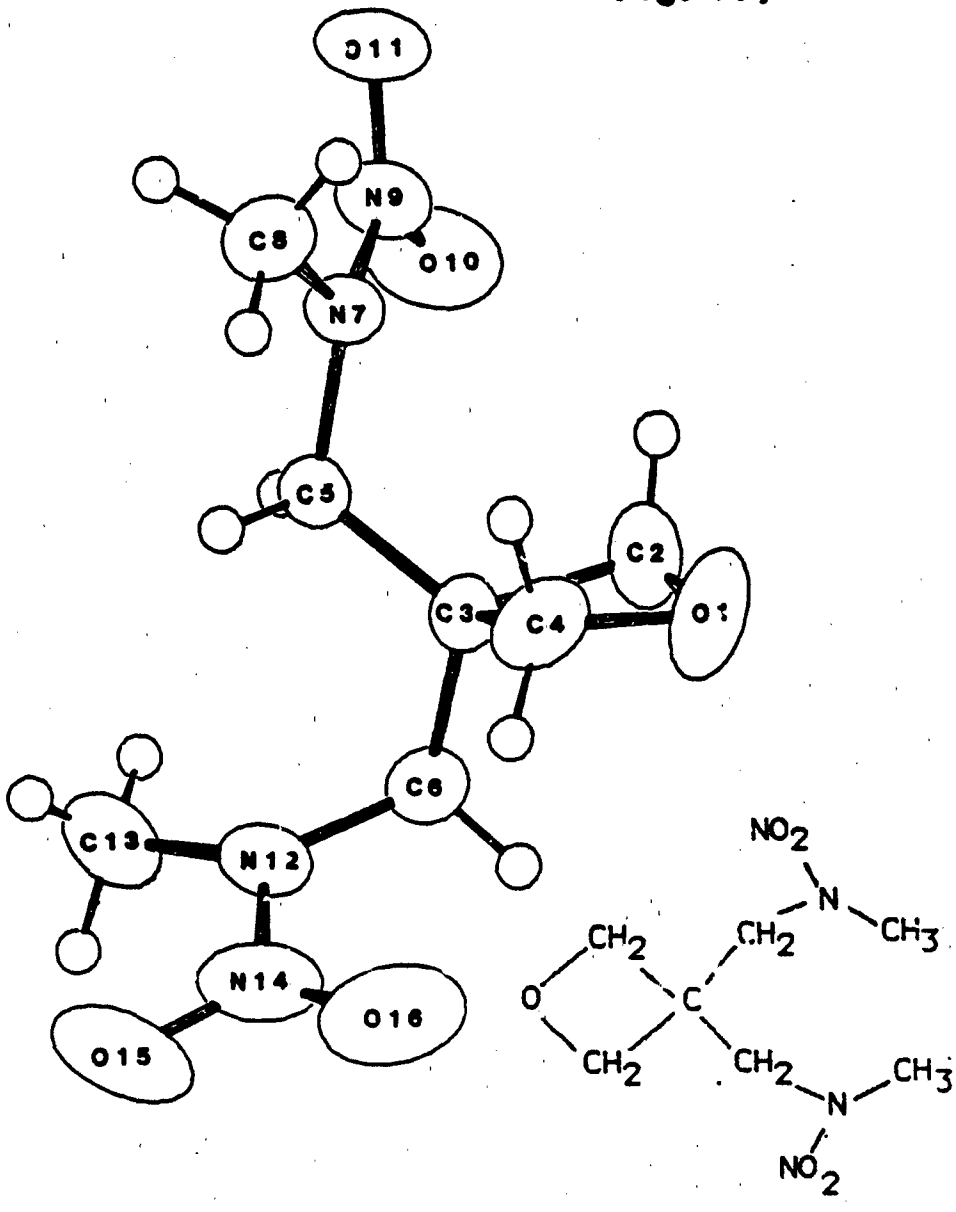
d = 1.573

f) 3,3-Bis(methylnitroaminomethyl)oxetane

Interest in this compound stems from its potential use as a monomeric precursor in producing energetic polymers or copolymers. Crystals of the monomer were provided by G. Manser of Morton Thiokol . The space group is monoclinic, $P2_1/c$, with unit cell a = 14.106(4)Å, b = 6.472(2)Å, c = 11.963(3)Å, and β =99.50(1)°, and a calculated density of 1.444 Mg mm^{-3}. Bond distances and angles are given in Table (7). Fig. (7) shows the molecular geometry and gives the numbering scheme. Table (7) also includes a selected set of torsion angles defining the geometry of the methylnitroaminomethyl arms. In this molecule the oxetane ring is puckered such that the dihedral angle between C(2)-C(3)-C(4) and the C(2)-O(1)-C(4) planes is 20.6°. Bonding for nitrogens N(7) and N(12) is pyramidal with the N-N vector making an angle of 22.6 and 13.6° with the N-C-C plane including the two methyl carbons.

Intermolecular contacts are at normal van der Waals seperations. Nearest contacts are O(16)—H(2B)' = 2.44Å, O(15)--H(6B)' = 2.63Å, O(1)—H(5B)' = 2.64Å, and H(13A)--H(13A)' = 2.58Å.

Fig. (7)



3,3-Bis(methylaminomethyl)oxetane

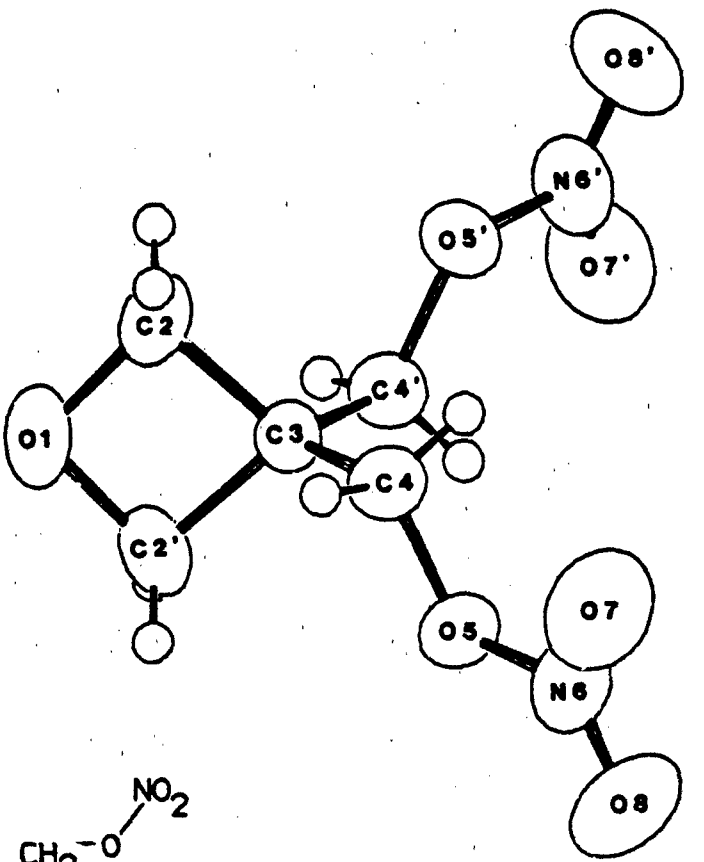
d = 1.444

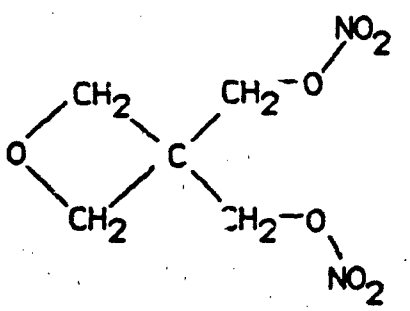
g) 3,3-Bis(nitratomethyl)oxetane

This energetic monomer, provided by G. Manser of Morton Thiokol, crystallizes in the space group C2/c with a = 15.120(4), b = 6.163(1), c = 12.958(4)Å, and β =132.76(2)°. The calculated density is 1.556 Mg mm^{-3}. The bond distances, angles, and a selected set of torsion angles are given in Table (8). Fig. (8), drawn from experimental coordinates, gives the atom numbering system. The molecule has C_2 symmetry about the cross ring O(1)—C(3) axis (coincident with the b crystal axis) so that only the unprimed atoms in Fig. (3) are independent. In this molecule the oxetane ring is planar. Orientation of the nitratomethyl arm with respect to the oxetane ring is defined by the torsion angles given in Table (8) as is the orientation of the nitrato group.

Intermolecular contacts are at normal van der Waals separations. Nearest contacts are H(4A)—O(8)' = 2.68Å, H(2B)—O(7)' = 2.71Å and O(8)—H(4B)' = 2.72Å.

Fig. (8)





3,3-Bis(nitratomethyl)oxetane

d = 1.556

h) 3-Methoxy-2,4-dinitro-2,4-diazapentane

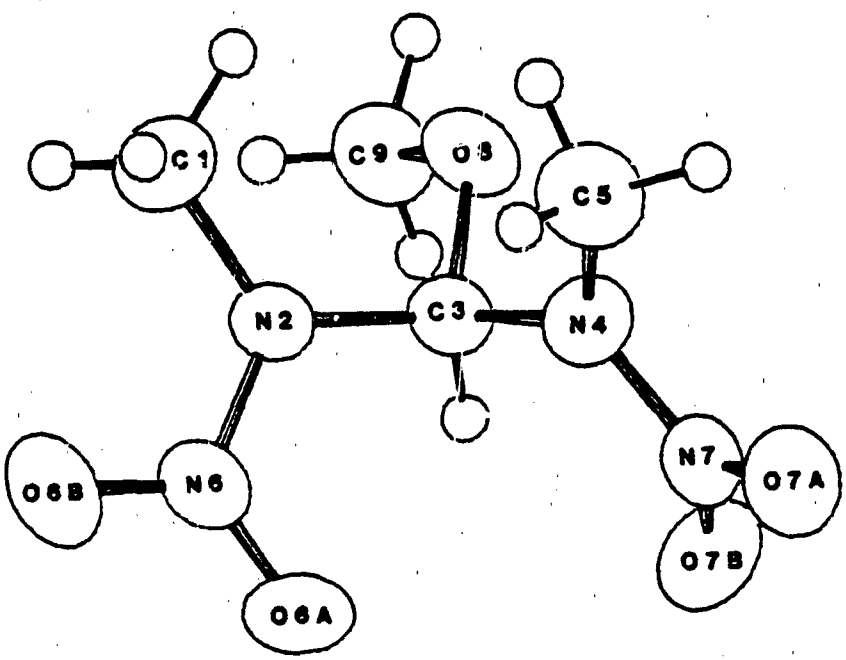
This compound was provided by H. Adolph of NSWC. The material crystallized in the monoclinic space group $P2_1/c$, a = 7.964(1), b = 8.320(1), c = 14.767(2)Å, and β = 119.73(1)°. The calculated density is 1.518 Mg mm^{-3}. Bond distances, angles, and torsion angles are given in Table (9), and the atom numbering is given in Fig. (9). In this compound the amino nitrogens are nearly planar. The N-N vector makes an angle of 1.0° at N(2) with the C(1)-N(2)-C(3) plane and 8.5° at N(4) with the C(5)-N(4)-C(3) plane.

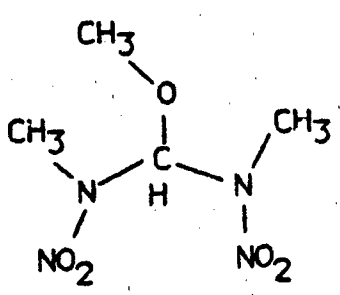
There are no unusual intermolecular contacts in this molecule. Nearest approaches are H(1A)---H(1A)' = 2.41(4)Å, O(6B)---H(9A)' = 2.57(3)Å, O(7A)---H(9A)' = 2.60(3)Å and H(9c)---O(6B)' = 2.64(3)Å.

i) Tribenzyltriazawurtzitane

This cage compound was provided by A. Nielson, China Lake. It is a possible precursor of the hypothetical target compound hexa-azahexanitrowurtzitane; the target compound is a higher mol. wt. analog of RDX which is predicted to be 5-10% denser than RDX. The precursor material crystallized in the monoclinic space group $P2_1/c$, with a = 10.968(1), b = 11.965(1), c = 18.857(2)Å, and β = 95.77(1)°. The calculated density is 1.175 Mg mm^{-3}. Bond distances and angles are given in Table (10). The crystal is disordered (contains two conformations of the molecule). The major conformer (70% occupancy) is shown in Fig. (10). In the minor conformer, benzyl ring C is rotated to an alternate position, C' (30% occupancy). In this compound the aza nitrogens are pyramidal with an average angle between the N-methylene carbon vector and the C-N-C ring plane of 40.8°; this is essentially tetrahedral (sp^3) geometry.

Fig. (9)

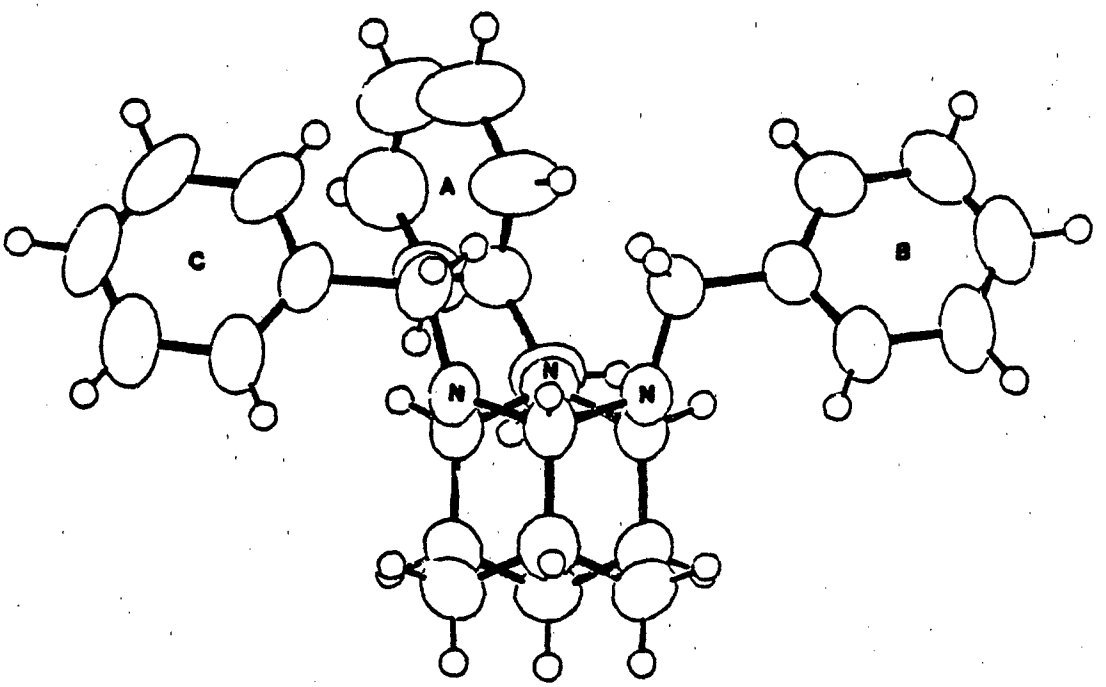


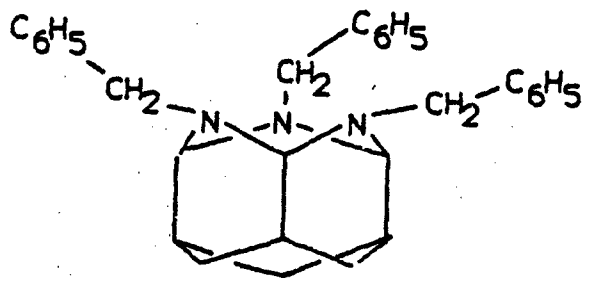


3-Methoxy-2,4-dinitro-2,4-diazapentane

d = 1.518

Fig. (10)





Tribenzyltriazawurtzitane

d = 1.175

j) 3-Cyano-4,4,5,5-tetramethylisoxazoline-N-oxide

Crystals of this material were provided by J. Boyer of the University of Illinois at Chicago. This compound was synthesized from a starting material which contained a cyclopropane ring (an energetic moiety). During the nitration reaction, the three-membered ring opens, and a five-membered ring forms, incorporating two atoms of the nitro group.

The compound crystallizes in the orthorhombic space group $Pna2_1$, a = 10.283(3), b = 12.389(4), and c = 7.262(3)Å. The calculated density is 1.207 Mg mm^{-3}. Bond distances and angles are given in Table (11) and the molecular geometry is illustrated in Fig. (11). The ring geometry is described by torsion angles O(1)-N(2)-N(3)-C(4) = 3.4(15)°, C(5)-C(4)-C(3)-N(2) = -20.6(1.3)°, and C(3)-N(2)-O(1)-C(5) = 16.1(1.4)°.

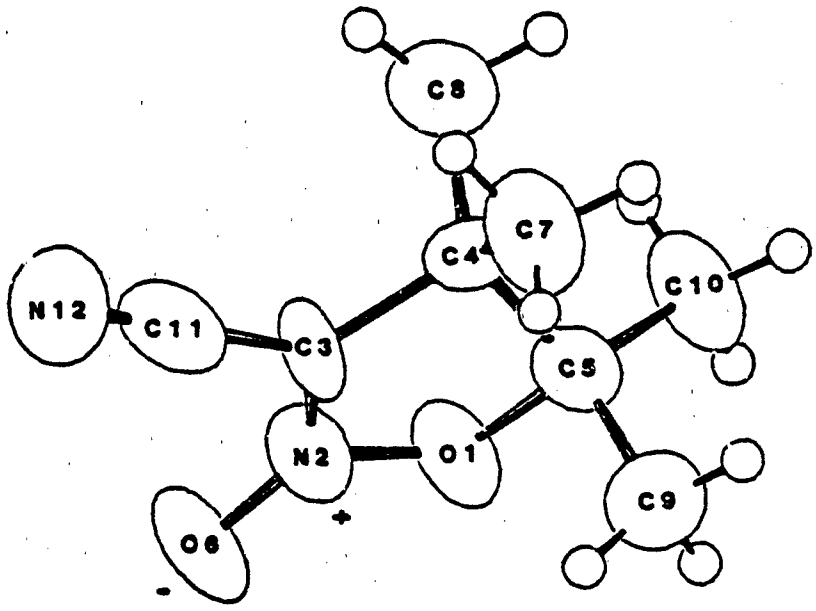
Intermolecular contacts at normal van der Waals seperations. Nearest contacts are O(6)--H(7A)' = 2.69Å.

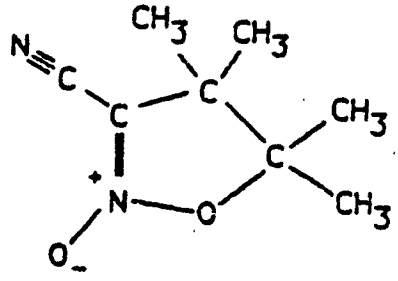
k) 5-Aza-6-methoxyuracil

Samples of this material were provided by C. Coon of Lawrence Livermore Laboratory. The material crystallized in the monoclinic space group $P2_1/c$, a = 9.994(5)Å. b = 4.316(1)Å, c = 15.891(8)Å, and β = 115.4(3)°. The calculated density is 1.557 Mg mm^{-3}. Bond distances and angles are given in Table (12) and the molecular geometry is shown in Fig. (12). The puckered triaza ring geometry is described by the selected list of torsion angles given in Table (12).

In this material each of the nitrogens participate in an intermolecular hydrogen bond; N(1) acts as a donor to O(6)', (1-x,y-.5,.5-z), N(3) is a donor to O(2)', (1-x,-y,-z), and N(5) is a donor to O(4)', (-x,y-.5,.5-z) The respective H--O', N--O' distances and N-H--O angle are; 2.08Å, 2.82Å, and 145.2°, 2.02Å, 2.86Å, and 166.3°, and 2.01Å, 2.81Å, and 157.2°.

Fig. (11)

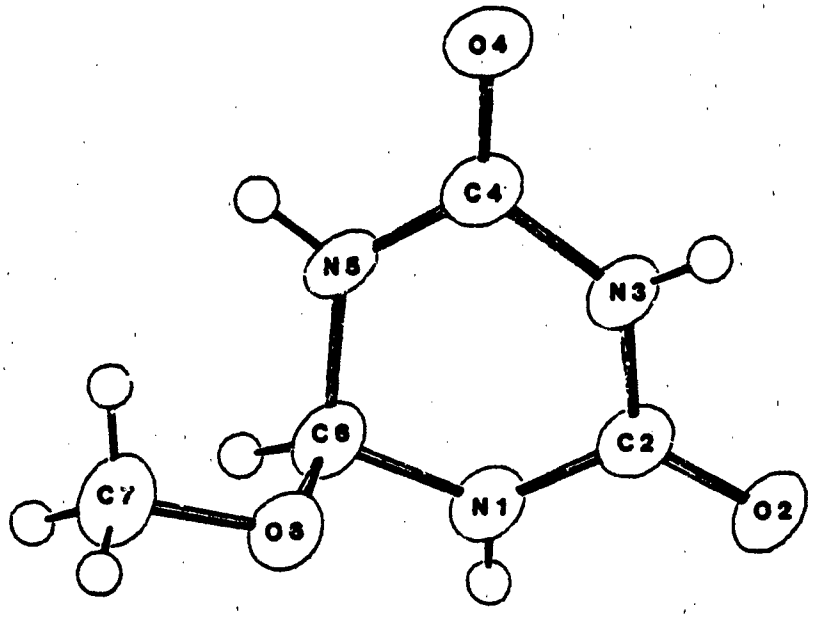


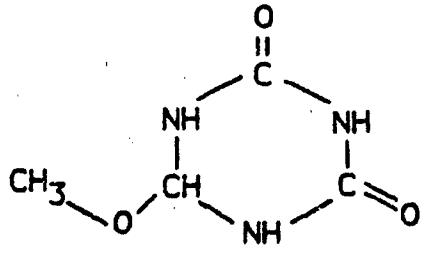


3-Cyano-4,4,5,5-tetramethylisoxazoline-N-oxide

d = 1.207

Fig. (12)





5-Aza-6-methoxyuracil

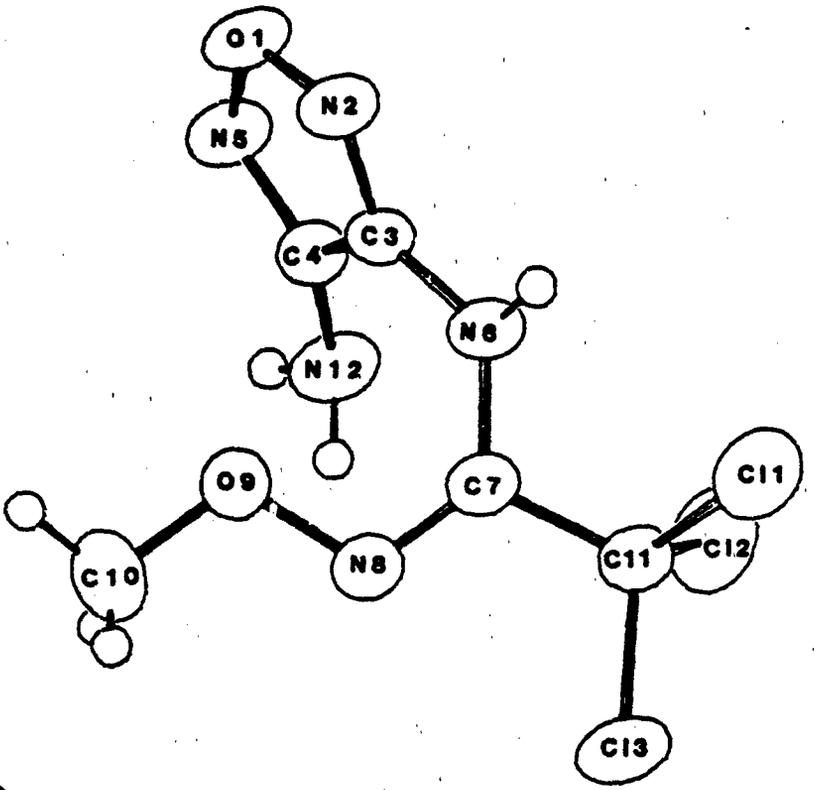
d = 1,557

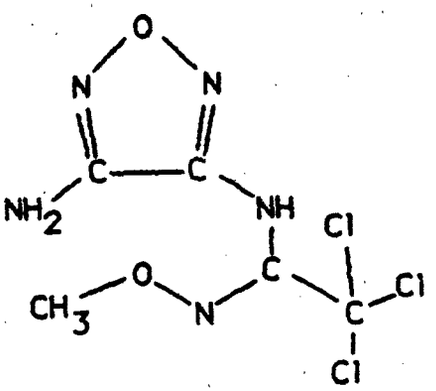
2) N-(4-amino-1,2,5-triazolo)-N'-methoxy-trichloroacetamidine

Crystals of this material, provided by C. Coon of Lawrence Livermore Laboratory, formed in the monoclinic space group $P2_1/c$, a = 9.287(1)Å, b = 9.493(1)Å, c = 13.208(2)Å, and β = 108.47(1)° with a calculated density of 1.494 Mg m^{-3}. Bond distances and angles are given in Table (13) as well as a selected set of torsion angles. Fig. (13) shows the molecular geometry and the atom numbering. In this compound the furazan ring is planar. Orientation of the methoxy and trichloracetamidine groups are described by the torsion angles given in Table (13).

There are no unusual intermolecular contacts, nearest contacts are N(2)—H(6)' = 2.30Å, H(12B)—N(5)' = 2.37Å, and H(12A)—N(8)' = 2.50Å.

Fig. (13)





N-(4-amino-1,2,5-triazolo)-N'-methoxy-trichloroacetamidine

d = 1.494

Appendix A

Table (1) Bond distances (A) and angles (deg.) for Tetra nitrobishomocubane with e.s.d.'s in parenthesis

	Molecule 1	Molecule 2
C(1)-C(4)	1.565(4)	1.564(4)
C(1)-C(6)	1.529(4)	1.529(4)
C(1)-C(9)	1.501(4)	1.516(4)
C(2)-C(3)	1.549(4)	1.552(4)
C(2)-C(7)	1.549(4)	1.554(4)
C(2)-C(9)	1.541(3)	1.524(4)
C(3)-C(4)	1.558(4)	1.561(4)
C(3)-C(10)	1.527(3)	1.519(3)
C(4)-C(5)	1.569(4)	1.571(4)
C(5)-C(6)	1.549(5)	1.547(4)
C(5)-C(8)	1.541(5)	1.535(5)
C(6)-C(7)	1.562(4)	1.569(4)
C(7)-C(8)	1.565(4)	1.566(4)
C(8)-C(10)	1.505(4)	1.504(4)
C(9)-N(1)	1.520(4)	1.517(4)
C(9)-N(2)	1.522(4)	1.521(4)
C(10)-N(3)	1.514(4)	1.534(4)
C(10)-N(4)	1.526(4)	1.513(4)
N(1)-O(1)	1.204(4)	1.196(5)
N(1)-O(2)	1.193(4)	1.202(5)
N(2)-O(3)	1.196(4)	1.188(5)
N(2)-O(4)	1.208(3)	1.175(4)
N(3)-O(5)	1.203(4)	1.181(4)
N(3)-O(6)	1.214(4)	1.187(4)
N(4)-O(7)	1.202(4)	1.202(4)
N(4)-O(8)	1.204(4)	1.206(4)
Bond angles		
C(4)-C(1)-C(6)	87.7(2)	87.5(2)
C(4)-C(1)-C(9)	103.8(2)	104.6(2)
C(6)-C(1)-C(9)	105.6(3)	104.8(3)
C(3)-C(2)-C(7)	99.7(2)	99.9(2)
C(3)-C(2)-C(9)	100.0(2)	101.4(2)
C(7)-C(2)-C(9)	104.2(2)	104.6(2)
C(2)-C(3)-C(4)	100.2(2)	100.0(2)
C(2)-C(3)-C(10)	103.3(2)	102.3(2)
C(4)-C(3)-C(10)	102.1(2)	102.5(2)
C(1)-C(4)-C(3)	105.2(2)	104.9(2)
C(1)-C(4)-C(5)	89.8(2)	90.2(2)
C(3)-C(4)-C(5)	103.7(2)	103.4(2)
C(4)-C(5)-C(6)	86.9(2)	86.6(2)
C(4)-C(5)-C(8)	103.0(2)	103.8(2)

	Molecule 1	Molecule 2
C(1)-C(6)-C(5)	91.9(2)	92.4(2)
C(1)-C(6)-C(7)	103.8(2)	104.1(2)
C(5)-C(6)-C(7)	87.0(2)	86.7(2)
C(2)-C(7)-C(6)	103.9(2)	102.9(2)
C(2)-C(7)-C(8)	105.5(2)	105.7(2)
C(6)-C(7)-C(8)	90.5(2)	90.3(2)
C(5)-C(8)-C(7)	87.2(2)	87.3(2)
C(5)-C(8)-C(10)	103.6(2)	103.6(2)
C(7)-C(8)-C(10)	106.1(2)	104.7(2)
C(1)-C(9)-C(2)	98.1(2)	97.7(2)
C(1)-C(9)-N(1)	113.4(3)	115.4(3)
C(1)-C(9)-N(2)	113.3(2)	111.2(2)
C(2)-C(9)-N(1)	112.3(2)	112.0(2)
C(2)-C(9)-N(2)	115.1(2)	114.8(3)
N(1)-C(9)-N(2)	104.9(2)	106.0(2)
C(3)-C(10)-C(8)	97.8(2)	99.0(2)
C(3)-C(10)-N(3)	112.4(2)	113.2(2)
C(3)-C(10)-N(4)	114.2(2)	111.6(2)
C(8)-C(10)-N(3)	112.7(2)	112.8(2)
C(8)-C(10)-N(4)	115.5(3)	115.7(2)
N(3)-C(10)-N(4)	104.6(2)	105.0(2)
O(1)-N(1)-C(9)	117.1(3)	117.3(3)
O(2)-N(1)-C(9)	117.7(3)	116.2(3)
O(1)-N(1)-O(2)	125.3(3)	126.5(3)
O(3)-N(2)-C(9)	116.0(2)	118.2(2)
O(4)-N(2)-C(9)	118.5(3)	117.7(3)
O(3)-N(2)-O(4)	125.4(3)	123.6(3)
O(5)-N(3)-C(10)	118.7(2)	118.2(2)
O(6)-N(3)-C(10)	116.8(3)	116.3(3)
O(5)-N(3)-O(6)	124.5(3)	125.4(3)
O(7)-N(4)-C(10)	117.8(3)	116.9(3)
O(8)-N(4)-C(10)	116.1(2)	117.6(2)
O(7)-N(4)-O(8)	126.1(3)	125.3(3)

ANPZ

Table 2. Bond Lengths and Corrections for Libration* (Å).

Bond	uncorrected	corrected
N(1) - C(2)	1.334(3)	1.337
N(1) - C(6)	1.336(3)	1.340
C(2) - C(3)	1.438(3)	1.444
C(5) - C(6)	1.439(3)	1.445
C(2) - N(7)	1.319(3)	1.323
C(6) - N(10)	1.326(3)	1.329
C(3) - N(4)	1.305(3)	1.309
C(5) - N(4)	1.311(3)	1.314
C(3) - N(8)	1.458(3)	1.462
C(5) - N(9)	1.441(3)	1.445
N(8) - O(11)	1.217(3)	1.247**
N(9) - O(14)	1.233(2)	1.264**
N(8) - O(12)	1.216(2)	1.247**
N(9) - O(13)	1.222(2)	1.253**

N(7) - H7A	0.82(3)	N(7) - H10A	0.89(3)
N(10)- H7B	0.78(3)	N(10)- H10B	0.80(3)

Hydrogen bonds - Intermolecular

N(10)..O(13)'	2.902(3)	H10A..O(13)'	2.02(3)
N(10)..O(12)'	2.986(3)	H10B..O(12)'	2.32(3)
N(7). .O(14)'	2.909(3)	H7A...O(14)'	2.32(3)
N(7)...O(12)"	3.221(3)	H7B...O(12)"	2.49(3)

Intramolecular

N(10)..O(14)	2.652(3)	H10B..O(14)	2.06(3)
N(7)...O(11)	2.673(3)	H7A...O(11)	2.10(3)

* The nitro oxygens did not fit an overall rigid-body model and their thermal factors were excluded from the libration/translation tensor determination. The method of Schomaker & Trueblood (1968) was used.

** Nitro distances corrected by assuming riding-motion correlation approximation (Johnson,1970).

Table 3. Bond Angles (degrees). All unstated estimated standard deviations are 0.2°. Values in left and right columns are related by non-crystallographic molecular symmetry.

C(2)C(3)N(4)	122.1	C(6)C(5)N(4)	121.9
N(4)C(3)N(8)	115.3	N(4)C(5)N(9)	115.6
C(2)C(3)N(8)	122.6	C(6)C(5)N(9)	122.5
N(1)C(2)N(7)	116.8	N(1)C(6)N(10)	116.8
C(3)C(2)N(7)	124.7	C(5)C(6)N(10)	124.8
N(1)C(2)C(3)	118.5	N(1)C(6)C(5)	118.4
O(12)N(8)O(11)	122.3	O(13)N(9)O(14)	121.9
O(12)N(8)C(3)	119.3	O(13)N(9)C(5)	120.1
O(11)N(8)C(3)	118.4	O(14)N(9)C(5)	118.0
C(2)N(1)C(6))	120.4		
C(3)N(4)C(5)	118.7		

Hydrogen Bond Angles

Intermolecular		Intramolecular	
N(10)H(10A)O13'	174(2)	N(10)H(10B)O(14)	130(2)
N(10)H(10B)O12'	141(2)	N(7)H(7A)O(11)	127(2)
N(7)H(7A)O14'	129(2)		
N(7)H(7B)O12"	156(3)		

Table (4). Bond distances (Å) and valence angles (deg.) for tetranitrobicyclooctane with e.s.d.'s in parentheses

Bond Distances (Å)	Molecule 1	Molecule 2	Disorder (Molecule 2)
C(1)-O(2)	1.423(4)	1.427(4)	-
O(2)-C(3)	1.413(4)	1.438(7)	1.360(17)
C(3)-C(4)	1.523(5)	1.538(6)	1.573(14)
C(4)-C(5)	1.520(6)	1.541(5)	-
C(5)-C(1)	1.524(4)	1.518(4)	-
C(5)-O(6)	1.430(4)	1.426(4)	-
O(6)-C(7)	1.420(5)	1.437(4)	-
C(7)-C(8)	1.521(4)	1.516(5)	-
C(8)-C(1)	1.529(5)	1.522(5)	-
C(4)-N(1)	1.508(5)	1.500(7)	1.563(13)
C(4)-N(2)	1.518(4)	1.481(6)	1.485(13)
C(8)-N(3)	1.522(5)	1.514(5)	-
C(8)-N(4)	1.505(5)	1.504(4)	-
N(1)-O(1A)	1.215(4)	1.195(8)	1.188(16)
N(1)-O(1B)	1.207(5)	1.192(11)	1.220(30)
N(2)-O(2A)	1.207(5)	1.215(7)	1.170(16)
N(2)-O(2B)	1.212(5)	1.215(9)	1.209(17)
N(3)-O(3A)	1.210(5)	1.199(5)	-
N(3)-O(3B)	1.215(5)	1.196(6)	-
N(4)-O(4A)	1.204(5)	1.216(5)	-
N(4)-O(4B)	1.210(5)	1.192(6)	-
Bond Angles (deg.)			
O(2)-C(1)-C(5)	107.3(2)	107.3(3)	-
C(5)-C(1)-C(8)	103.1(3)	103.1(3)	-
O(2)-C(1)-C(8)	109.4(3)	109.2(3)	-
C(1)-O(2)-C(3)	111.5(3)	110.9(3)	-
O(2)-C(3)-C(4)	104.5(3)	103.0(4)	104.9(10)
C(3)-C(4)-C(5)	104.2(3)	102.5(3)	102.0(7)
C(1)-C(5)-C(4)	103.2(3)	103.3(2)	-
C(1)-C(5)-O(6)	107.3(3)	107.7(3)	-
C(4)-C(5)-O(6)	109.3(2)	109.7(3)	-
C(5)-O(6)-C(7)	111.1(3)	110.1(2)	-
O(6)-C(7)-C(8)	104.4(3)	103.9(3)	-
C(1)-C(8)-C(7)	103.9(3)	103.7(3)	-
C(3)-C(4)-N(1)	109.9(3)	108.8(4)	107.8(3)
C(3)-C(4)-N(2)	114.8(3)	116.3(4)	113.7(8)
C(5)-C(4)-N(1)	111.4(3)	113.6(4)	109.9(5)
C(5)-C(4)-N(2)	110.8(3)	111.0(3)	116.4(6)
N(1)-C(4)-N(2)	105.8(3)	105.0(4)	106.8(7)
C(1)-C(8)-N(3)	110.1(3)	111.4(3)	-
C(1)-C(8)-N(4)	112.1(3)	111.1(3)	-
C(7)-C(8)-N(3)	110.4(3)	110.3(3)	-
C(7)-C(8)-N(4)	114.7(3)	114.2(3)	-
N(3)-C(8)-N(4)	105.7(3)	106.1(3)	-
C(4)-N(1)-O(1A)	114.4(3)	115.8(5)	117.6(12)

C(4)-N(1)-O(1B)	118.7(3)	117.8(8)	115.4(18)
O(1A)-N(1)-O(1B)	126.7(4)	126.2(9)	126.9(20)
C(4)-N(2)-O(2A)	117.9(3)	116.9(5)	112.9(14)
C(4)-N(2)-O(2B)	115.9(3)	120.2(5)	112.1(10)
O(2A)-N(2)-O(2B)	126.1(3)	122.9(6)	134.8(17)
C(8)-N(3)-O(3A)	118.7(3)	116.9(3)	-
C(8)-N(3)-O(3B)	115.1(3)	117.1(4)	-
O(3A)-N(3)-O(3B)	126.2(4)	126.0(4)	-
C(8)-N(4)-O(4A)	117.1(3)	115.1(4)	-
C(8)-N(4)-O(4B)	116.5(3)	118.4(3)	-
O(4A)-N(4)-O(4B)	126.4(4)	126.4(4)	-

Table (5). Bond distances (Å) and valence angles (deg.) for 2,3,4-trinitropyrrole with e.s.d.'s in parentheses

Bond Distance (Å)	Molecule (1)	Molecule (2)	Average
N(1)-C(2)	1.360(9)	1.386(10)	1.373
C(2)-C(3)	1.367(9)	1.383(9)	1.375
C(3)-C(4)	1.379(9)	1.423(10)	1.401
C(4)-C(5)	1.393(10)	1.351(11)	1.372
C(5)-N(1)	1.351(10)	1.339(10)	1.345
C(2)-N(6)	1.378(9)	1.434(9)	1.406
C(3)-N(7)	1.429(9)	1.461(8)	1.445
C(4)-N(8)	1.429(9)	1.430(9)	1.430
N(6)-O(6A)	1.198(8)	1.238(8)	1.218
N(6)-O(6B)	1.265(8)	1.148(8)	1.207
N(7)-O(7A)	1.249(8)	1.181(8)	1.215
N(7)-O(7B)	1.182(8)	1.216(8)	1.199
N(8)-O(8A)	1.180(8)	1.252(8)	1.216
N(8)-O(8B)	1.210(8)	1.233(8)	1.222
Bond Angles (deg.)			
C(2)-N(1)-C(5)	109.2(6)	108.3(6)	108.8
N(1)-C(2)-C(3)	108.7(6)	108.9(6)	108.8
C(2)-C(3)-C(4)	106.7(6)	104.4(6)	105.6
C(3)-C(4)-C(5)	108.3(6)	109.0(6)	108.7
C(4)-C(5)-N(1)	106.5(7)	108.8(7)	107.7
N(1)-C(2)-N(6)	119.4(6)	124.3(6)	121.8
C(3)-C(2)-N(6)	131.8(6)	126.8(6)	129.3
C(2)-C(3)-N(7)	124.9(6)	127.1(6)	126.0
C(4)-C(3)-N(7)	128.4(6)	128.2(6)	128.3
C(3)-C(4)-N(8)	127.5(6)	125.7(7)	126.6
C(5)-C(4)-N(8)	124.0(6)	125.0(7)	124.5
C(2)-N(6)-O(6A)	121.7(6)	115.6(6)	118.7
C(2)-N(6)-O(6B)	115.5(6)	117.7(6)	116.6
C(3)-N(7)-O(7A)	116.7(6)	119.2(5)	117.9
C(3)-N(7)-O(7B)	121.0(6)	113.3(5)	117.2
C(4)-N(8)-O(8A)	119.2(6)	117.2(6)	118.2
C(4)-N(8)-O(8B)	117.6(6)	117.8(6)	117.7
O(6A)-N(6)-O(6B)	122.8(6)	126.7(7)	124.8
O(7A)-N(7)-O(7B)	122.4(6)	127.5(6)	124.9
O(8A)-N(8)-O(8B)	123.1(6)	124.9(6)	124.0

Table (6). Bond distances Å and angles for 1,3,5-Trinitroso-1,3,5-triazacyclohexane

N(1)-C(2)	1.428(3)	N(5)-N(11)	1.367(14)
N(1)-C(6)	1.460(3)	N(5)-N(11A)	1.357(11)
N(1)-N(7)	1.333(3)	N(5)-N(11B)	1.382(13)
C(2)-N(3)	1.431(4)	N(7)-O(8)	1.179(4)
N(3)-C(4)	1.444(4)	N(9)-O(10)	1.209(4)
N(3)-N(9)	1.352(4)	N(11)-O(12)	1.207(18)
C(4)-N(5)	1.444(5)	N(11A)-O(12A)	1.211(14)
N(5)-C(6)	1.449(4)	N(11B)-O(12B)	1.211(29)

Bond Angles

C(2)-N(1)-C(6)	117.7(2)	C(4)-N(5)-N(11B)	135.8(9)
C(2)-N(1)-C(7)	124.1(2)	C(6)-N(5)-N(11)	107.5(7)
C(6)-N(1)-N(7)	124.1(2)	C(6)-N(5)-N(11A)	144.2(5)
N(1)-C(2)-N(3)	109.0(2)	C(6)-N(5)-N(11B)	105.9(9)
C(2)-N(3)-C(4)	116.8(2)	N(1)-C(6)-N(5)	106.7(2)
C(2)-N(3)-N(9)	116.7(2)	N(1)-N(7)-O(8)	115.6(3)
C(4)-N(3)-N(9)	125.6(2)	N(3)-N(9)-O(10)	113.4(3)
N(3)-C(4)-N(5)	108.5(2)	N(5)-N(11)-O(12)	107.3(14)
C(4)-N(5)-C(6)	117.6(3)	N(5)-N(11A)-O(12A)	105.6(10)
C(4)-N(5)-N(11)	133.9(8)	N(5)-N(11B)-O(12B)	108.1(13)
C(4)-N(5)-N(11A)	98.1(5)		

Table (7). Bond distances (Å) and valence angles for 3,3-Bis (methylnitroaminomethyl) oxetane with e.s.d.'s in parentheses

Bond Lengths (Å)

O(1)-C(2)	1.443(3)	O(1)-C(4)	1.431(3)
C(2)-C(3)	1.531(3)	C(3)-C(4)	1.542(3)
C(3)-C(5)	1.515(2)	C(3)-C(6)	1.525(2)
C(5)-N(7)	1.462(2)	C(6)-N(12)	1.456(2)
N(7)-C(8)	1.447(2)	N(7)-N(9)	1.336(2)
N(9)-O(10)	1.231(2)	N(9)-O(11)	1.228(2)
N(12)-C(13)	1.452(3)	N(12)-N(14)	1.336(2)
N(14)-O(15)	1.235(3)	N(14)-O(16)	1.223(3)

Bond Angles (deg.)

C(2)-O(1)-C(4)	90.8(2)	O(1)-C(2)-C(3)	91.0(2)
C(2)-C(3)-C(4)	83.5(1)	C(2)-C(3)-C(5)	119.9(2)
C(4)-C(3)-C(5)	118.3(1)	C(2)-C(3)-C(6)	109.3(1)
C(4)-C(3)-C(6)	113.4(1)	C(5)-C(3)-C(6)	110.1(1)
O(1)-C(4)-C(3)	90.9(2)	C(3)-C(5)-N(7)	115.0(1)
C(3)-C(6)-N(12)	114.8(1)	C(5)-N(7)-C(8)	121.2(1)
C(5)-N(7)-N(9)	117.3(1)	C(8)-N(7)-N(9)	116.8(1)
N(7)-N(9)-O(10)	118.1(2)	N(7)-N(9)-O(11)	117.9(1)
O(10)-N(9)-O(11)	123.9(2)	C(6)-N(12)-C(13)	122.2(2)
C(6)-N(12)-N(14)	120.2(2)	C(13)-N(12)-N(14)	115.9(2)
N(12)-N(14)-O(15)	117.8(2)	N(12)-N(14)(-O(16)	117.9(2)
O(15)-N(14)-O(16)	124.3(2)		

Torsion Angles (deg.)

C(2)-C(3)-C(5)-N(7)	-43.8(2)	C(5)-N(7)-N(9)-O(10)	-17.6(2)
C(6)-C(3)-C(5)-N(7)	-171.9(1)	C(6)-N(12)-N(14)-O(16)	7.5(2)
C(4)-C(3)-C(6)-N(12)	83.1(2)	C(3)-C(6)-N(12)-C(13)	94.2(2)
C(5)-C(3)-C(6)-N(12)	-52.0(2)	C(3)-C(5)-N(7)-C(8)	-105.2(2)

Table (8). Bond distances (Å) and valence angles for 3,3-Bis(nitratomethyl)oxetane with e.s.d.'s in parentheses

Bond Lengths (Å)		Bond Angles (deg.)	
O(1)-C(2)	1.437(2)	C(2)-O(1)-C(2)'	91.6(2)
C(2)-C(3)	1.532(2)	O(1)-C(2)-C(3)	91.9(2)
C(3)-C(4)	1.514(3)	C(2)-C(3)-C(2)'	84.5(2)
C(4)-C(5)	1.454(2)	C(2)-C(3)-C(4)	115.9(1)
O(5)-N(6)	1.386(3)	C(4)-C(3)-C(4)'	112.0(2)
N(6)-O(7)	1.181(3)	C(3)-C(4)-O(5)	104.2(1)
N(6)-O(8)	1.196(2)	C(4)-O(5)-N(6)	113.7(1)
		O(5)-N(6)-O(7)	119.6(2)
		O(5)-N(6)-O(8)	111.2(2)
		O(7)-N(6)-O(8)	129.2(3)

Torsion Angles (deg.)			
C(4)-C(3)-C(2)-O(1)	113.0(2)	C(4)-O(5)-N(6)-O(7)	-0.1(3)
C(2)-C(3)-C(4)-O(5)	62.3(2)	C(4)-O(5)-N(6)-O(8)	179.6(3)
N(6)-O(5)-C(4)-C(3)	172.7(2)		

Table (9). Bond distances (Å) and valence angles (deg.) for 3-Methoxy-2,4-dinitro-2,4-diazapentane.

Bond Lengths (Å)			
C(1)-N(2)	1.451(3)	N(2)-C(3)	1.466(2)
N(2)-N(6)	1.350(3)	C(3)-N(4)	1.446(2)
C(3)-O(8)	1.385(2)	N(4)-C(5)	1.446(2)
N(4)-N(7)	1.356(2)	N(6)-O(6A)	1.223(2)
N(6)-O(6B)	1.228(2)	N(7)-O(7B)	1.221(2)
N(7)-O(7A)	1.225(2)	O(8)-C(9)	1.440(2)

Bond Angles (deg.)			
C(1)-N(2)-C(3)	125.2(2)	C(1)-N(2)-N(6)	117.9(2)
C(3)-N(2)-N(6)	116.9(1)	N(2)-C(3)-N(4)	110.8(1)
N(2)-C(3)-O(8)	109.3(1)	N(4)-C(3)-O(8)	107.2(1)
C(3)-N(4)-C(5)	122.4(1)	C(3)-N(4)-N(7)	118.3(1)
C(5)-N(4)-N(7)	118.8(1)	N(2) N(6)-O(6A)	118.1(2)
N(2)-N(6)-O(6B)	117.2(1)	O(6A)-N(6)-O(6B)	124.7(2)
N(4)-N(7)-O(7B)	118.6(1)	N(4)-N(7)-O(7A)	116.7(1)
O(7B)-N(7)-O(7A)	124.7(1)	C(3)-O(8)-C(9)	112.8(1)

Torsion Angles			
C(1)-N(2)-C(3)-N(4)	93.4(2)	N(2)-C(3)-N(4)-N(7)	117.4(2)
C(1)-N(2)-C(3)-O(8)	-24.5(2)	O(8)-C(3)-N(4)-C(5)	66.2(2)
N(6)-N(2)-C(3)-N(4)	-85.6(2)	O(8)-C(3)-N(4)-N(7)	-123.4(2)
N(6)-N(2)-C(3)-O(8)	156.4(2)	N(2)-C(3)-O(8)-C(9)	-78.4(1)
C(1)-N(2)-N(6)-O(6A)	-177.2(1)	N(4)-C(3)-O(8)-C(9)	161.5(1)
C(1)-N(2)-N(6)-O(6B)	3.2(2)	C(3)-N(4)-N(7)-O(7B)	15.1(3)
C(3)-N(2)-N(6)-O(6A)	2.0(2)	C(3)-N(4)-N(7)-O(7A)	-165.8(2)
C(3)-N(2)-N(6)-O(6B)	-177.7(1)	C(5)-N(4)-N(7)-O(7B)	-174.2(2)
N(2)-C(3)-N(4)-C(5)	-52.9(2)	C(5)-N(4)-N(7)-O(7A)	4.9(3)

Table (10). Bond distances (Å) and valence angles (deg.) for tribenzyltriazawurtzitane with e.s.d.'s in parentheses

Bond Distances (Å)

N(1)-C(2)	1.1463(2)		C(8)-C(9)		1.515(3)
N(1)-C(6)	1.471(2)		C(9)-C(10)		1.523(3)
C(2)-N(3)	1.466(2)		C(10)-C(11)		1.528(3)
C(2)-C(9)	1.563(3)		C(11)-C(12)		1.525(3)
N(3)-C(4)	1.467(2)		N(1)-C(7A)		1.449(2)
C(4)-N(5)	1.459(2)		N(3)-C(7B)		1.448(2)
C(4)-C(11)	1.568(3)		N(5)-C(7C)		1.453(2)
N(5)-C(6)	1.469(2)		C(7A)-C(1A)		1.515(3)
C(6)-C(7)	1.566(3)		C(7B)-C(1B)		1.505(3)
C(7)-C(8)	1.530(3)		C(7C)-C(1C)		1.557(3)
C(7)-C(12)	1.516(3)		C(7C')-C(1C')		1.414(6)
	C(1)-C(2)		1.381(3)		1.369(3)
Benzene	C(1)-C(6)		1.381(3)		1.378(3)
ring	C(2)-C(3)	Ring A	1.373(3)	Ring B	1.387(4)
distances	C(3)-C(4)		1.368(4)		1.383(5)
	C(4)-C(5)		1.367(4)		1.355(5)
	C(5)-C(6)		1.392(4)		1.371(4)

* Rings C and C' fixed at C-C 1.395 and C-C-C = 120°.

Bond Angles (deg.)

C(2)-N(1)-C(6)	108.4(1)	N(5)-C(6)-C(7)	107.5(1)
C(2)-N(1)-C(7A)	113.6(1)	C(6)-C(7)-C(8)	110.0(1)
C(6)-N(1)-C(7A)	116.8(1)	C(6)-C(7)-C(12)	110.0(2)
N(1)-C(2)-N(3)	108.2(1)	C(8)-C(9)-C(12)	108.7(2)
N(1)-C(2)-C(9)	108.1(1)	C(7)-C(8)-C(9)	107.5(2)
N(3)-C(2)-C(9)	114.6(1)	C(2)-C(9)-C(8)	110.0(2)
C(2)-N(3)-C(4)	108.8(1)	C(2)-C(9)-C(10)	109.7(2)
C(2)-N(3)-C(7B)	118.8(1)	C(8)-C(9)-C(10)	109.0(2)
C(4)-N(3)-C(7B)	117.7(1)	C(9)-C(10)-C(11)	107.3(2)
N(3)-C(4)-N(5)	109.1(1)	C(4)-C(11)-C(10)	110.6(2)
N(3)-C(4)-C(11)	113.4(1)	C(4)-C(11)-C(12)	109.4(2)
N(5)-C(4)-C(11)	108.1(1)	C(10)-C(11)-C(12)	108.7(2)
C(4)-N(5)-C(6)	108.3(1)	C(7)-C(12)-C(11)	107.6(2)
C(4)-N(5)-C(7C)	113.7(1)	N(1)-C(7A)-C(1A)	111.7(1)
C(6)-N(5)-C(7C)	116.5(1)	N(3)-C(7B)-C(1B)	113.1(2)
N(1)-C(6)-N(5)	115.3(1)	N(5)-C(7C)-C(1C)	108.1(2)
N(1)-C(6)-C(7)	107.7(1)	N(5)-C(7C)-C(1C')	121.9(3)

Table (11). Bond distances (Å) and valence angles for 3-Cyano-4,4,5,5-tetramethylisoxazoline-N-oxide with e.s.d.'s in parentheses

Bond distances (Å)

O(1)-N(2)	1.390(15)	C(4)-C(5)	1.532(16)
O(1)-C(5)	1.511(15)	C(4)-C(7)	1.552(16)
N(2)-C(3)	1.302(18)	C(4)-C(8)	1.520(14)
N(2)-O(6)	1.238(15)	C(5)-C(9)	1.480(19)
C(3)-C(4)	1.511(17)	C(5)-C(10)	1.539(16)
C(3)-C(11)	1.416(20)	C(11)-N(12)	1.148(21)

Bond Angles (deg.)

N(2)-O(1)-C(5)	105.4(9)	C(5)-C(4)-C(7)	111.4(8)
O(1)-N(2)-C(3)	111.5(11)	C(5)-C(4)-C(8)	114.9(9)
O(1)-N(2)-O(6)	117.8(10)	C(7)-C(4)-C(8)	109.9(9)
C(3)-N(2)-O(6)	130.7(12)	C(4)-C(5)-O(1)	103.0(11)
N(2)-C(3)-C(4)	112.1(11)	C(4)-C(5)-C(9)	116.6(10)
N(2)-C(3)-C(11)	120.4(13)	C(4)-C(5)-C(10)	117.1(11)
C(4)-C(3)-C(11)	127.2(11)	O(1)-C(5)-C(9)	104.3(10)
C(3)-C(4)-C(5)	98.9(9)	O(1)-C(5)-C(10)	102.7(9)
C(3)-C(4)-C(7)	112.0(9)	C(9)-C(5)-C(10)	110.7(12)
C(3)-C(4)-C(8)	109.3(7)	C(3)-C(11)-N(12)	179.0(15)

Table (12). Bond distances (Å) and valence angles for 5-aza-6-methoxyuracile with e.s.d.'s in parentheses

Bond Distance (Å)

N(1)-C(2)	1.352(4)	C(4)-N(5)	1.350(5)
N(1)-C(6)	1.435(5)	C(4)-O(4)	1.277(5)
C(2)-N(3)	1.366(5)	N(5)-C(6)	1.424(5)
C(2)-O(2)	1.225(3)	C(6)-O(6)	1.428(4)
N(3)-C(4)	1.374(4)	O(6)-C(7)	1.445(3)

Bond Angles (deg.)

C(2)-N(1)-C(6)	121.7(3)	O(4)-C(4)-N(5)	124.1(3)
N(1)-C(2)-N(3)	115.1(2)	C(4)-N(5)-C(6)	122.4(3)
N(1)-C(2)-O(2)	122.1(3)	N(1)-C(6)-N(5)	109.4(3)
O(2)-C(2)-N(3)	122.7(3)	N(1)-C(6)-O(6)	107.1(3)
C(2)-N(3)-C(4)	125.2(3)	N(5)-C(6)-O(6)	112.4(3)
N(3)-C(4)-N(5)	114.5(3)	C(6)-O(6)-C(7)	113.8(2)
N(3)-C(4)-O(4)	121.4(3)		

Torsion Angles

N(1)-C(6)-N(5)-C(4)	-36.5(4)	O(2)-C(2)-N(3)-C(4)	167.4(3)
O(6)-C(6)-N(5)-C(4)	82.4(3)	C(2)-N(3)-C(4)-N(5)	11.0(5)
N(5)-C(6)-O(6)-C(7)	69.4(3)	N(3)-C(4)-N(6)-C(6)	15.5(4)
C(6)-N(1)-C(2)-N(3)	-13.9(5)		

Table (13). Bond distances (Å) and valence angles (deg.) for N-(4-amino-1,2,5-triazolo)-N'-methoxy-trichloroacetamidine with e.s.d.'s in parentheses

Bonds Distances (Å)

O(1)-N(2)	1.382(3)	C(7)-C(11)	1.525(5)
O(1)-N(5)	1.402(3)	C(8)-O(9)	1.396(4)
N(2)-C(3)	1.301(4)	O(9)-C(10)	1.411(5)
C(3)-C(4)	1.435(4)	C(11)-CL(1)	1.766(3)
C(3)-N(6)	1.377(4)	C(11)-CL(2)	1.768(3)
C(4)-N(5)	1.306(4)	C(11)-CL(3)	1.752(3)
C(4)-N(12)	1.360(4)		
N(6)-C(7)	1.3[illegible](4)		
C(7)-N(8)	1.273(4)		

Bond Angles (deg.)

N(5)-O(1)-N(2)	110.2(2)	C(7)-N(8)-O(9)	110.8(2)
O(1)-N(2)-C(3)	106.1(2)	N(8)-O(9)-C(10)	110.6(3)
N(2)-C(3)-C(4)	109.4(3)	C(7)-C(11)-CL(1)	110.2(2)
N(2)-C(3)-N(6)	121.6(2)	C(7)-C(11)-CL(2)	108.5(2)
C(4)-C(3)-N(6)	128.7(3)	C(7)-C(11)-CL(3)	111.7(3)
C(3)-C(4)-N(5)	108.7(2)	CL(1)-C(11)-CL(2)	108.7(2)
C(3)-C(4)-N(12)	128.1(3)	CL(2)-C(11)-CL(3)	109.1(2)
N(5)-C(4)-N(12)	123.1(3)	CL(3)-C(11)-CL(1)	108.4(2)
C(4)-N(5)-O(1)	105.7(2)		
C(3)-N(6)-C(7)	124.3(3)		
N(6)-C(7)-N(8)	127.6(3)		
N(6)-C(7)-C(11)	115.0(3)		
N(8)-C(7)-C(11)	117.2(3)		

Torsion Angles

O(1)-N(2)-C(3)-N(6)	172.7(3)	C(3)-N(6)-C(7)-C(11)	147.1(3)
C(7)-N(6)-C(3)-C(4)	-44.0(5)	N(6)-C(7)-N(8)-O(9)	-5.2(4)
C(3)-N(6)-C(7)-N(8)	-29.0(5)	C(11)-C(7)-N(8)-O(9)	178.8(2)

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